

Multiscale Splitting method for Boltzmann-Poisson Equation: Application for Dynamic of Electrons

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January 13, 2012

Abstract

In this paper we present a model based on dynamics of the electrons in the plasma using a simplified Boltzmann equation coupled with a Poisson equation.

The motivation arose to simulate active plasma resonance spectroscopy which is used for plasma diagnostic techniques, see [2], [14] and [16].

We are interested on designing splitting methods to the model problem.

First we reduce to a simplified transport equation and start to analyze the abstract Cauchy problem based on semi-groups.

Second we extent to the coupled transport and kinetic model and apply the splitting ideas.

The results are discussed with first numerical experiments to give discuss the numerical methods.

Keywords: kinetic model, neutron transport, dynamics of electrons, transport equation, splitting schemes, semi-group.

AMS subject classifications. 35K25, 35K20, 74S10, 70G65.

1 Introduction

We motivate our studying on simulating a active plasma resonance spectroscopy, which is well established in plasma diagnostic techniques.

To study the model with simulation models, we concentrate on an abstract kinetic model, which described the dynamics of electrons in the plasma by using a Boltzmann equation. The Boltzmann equation is coupled with the electric field and we obtain coupled partial differential equations.

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Our combined model is done simplified to apply with functional analytical tools. We discuss the description of a positive semi-group, which helps to do the numerical estimations in the splitting schemes.

Second a numerical method is discussed with respect to separate differential and integral part of the equations.

The numerical approximation is done by applying splitting methods of second order.

The paper is outlined as follows.

In section 2 we present our mathematical model and a possible reduced model for the further approximations.

The functional analytical setting with semi-groups are discussed in section 3. The splitting schemes are presented in in Section 4 and the numerical integration of the integro-part is discussed in Section 5.

Numerical experiments are done in Section 6. In the contents, that are given in Section 7, we summarize our results.

2 Mathematical Model

In the following a model is presented due to the motivation in [2], [14] and [16].

The models consider a fluid dynamical approach of the natural ability of plasmas to resonate in the near of the electron plasma frequency ω_{pe} .

Here we specialize to an abstract kinetic model to describe the dynamics of the electrons in the plasma, that allows to do the resonance-analysis.

The Boltzmann equation for the electron particles are given as

$$\begin{aligned} \frac{\partial f(x, v, t)}{\partial t} &= -v \cdot \nabla_x f(x, v, t) - \frac{e}{m_e} \nabla_x \phi \cdot \nabla_v f(x, v, t) \\ &\quad - \sigma(x, v, t) f(x, v, t) + \int_V \kappa(x, v, v') f(x, v', t) dv', \\ f(x, v, 0) &= f_0(x, v), \end{aligned} \tag{1}$$

and boundary conditions are postulated at the boundaries of P (plasma).

In front of the materials we assume complete reflection of the electrons due to the sheath $f(v_{||} + v_{\perp})$ with $v_{||}$ is the parallel and v_{\perp} perpendicular to the surface normal vector. ϕ is the electric field.

The Boltzmann's equation has to be coupled with the electric field. The electrostatic approximation of the field is represented by the potential that is valid on the complete volume S .

We apply the the Poisson's equation:

$$-\nabla_x \cdot (\epsilon \nabla \phi) = \begin{cases} e(n_i - \int f dS) & \text{in } P \\ 0 & \text{in } D \end{cases}, \tag{3}$$

the permittivity is equal to ϵ_0 in the plasma P and $\epsilon_0 \epsilon_D$ in the dielectric D . ϕ fulfills the boundary conditions U_n at any electrode E_n and $-\mathbf{n} \cdot \nabla \phi = 0$ at isolator I , whereas \mathbf{n} is the normal vector of the isolator surface.

On the surface of the dielectric a surface charge σ may accumulate and leads to a transition condition:

$$\Delta(\epsilon \nabla \phi) = -\sigma. \quad (4)$$

3 Semi-groups for Transport Equations

In the following, we derive the exponential growth of the transport semi-groups that is used in the section of the numerical methods.

We discuss in the following subsections two directions of the transport regimes:

- Neutron transport and
- Electron transport.

3.1 Transport model for the neutrons

For this model we can assume that $f(x, v, t)$ describe the density distribution of particles at position $x \in S$ with speed $v \in V$ at time $t \in [0, T]$, see also [4] and [17].

The space S is assumed to be a compact and convex subset of \mathbb{R}^3 with nonempty interior, and the velocity space V is:

$$V := \{v \in \mathbb{R}^3 : v_{min} \leq ||v||_2 \leq v_{max}\}$$

for $v_{min} > 0$ and $v_{max} < \infty$.

Assumption 3.1. *We have the following assumptions:*

- *Particles move according to their speed v .*
- *Particles are absorbed with function σ (e.g. probability function), depending on x and v .*
- *Particles are scattered to a scattering kernel κ depending on position x , incoming speed v' and outgoing speed v .*

The neutron transport is given as:

$$\begin{aligned} \frac{\partial f(x, v, t)}{\partial t} &= -v \cdot \nabla f(x, v, t) - \sigma(x, v, t)f(x, v, t) \\ &+ \int_V \kappa(x, v, v')f(x, v', t) dv', \end{aligned} \quad (5)$$

$$f(x, v, 0) = f_0(x, v), \quad (6)$$

and boundary conditions are included in the transport operator A_0 see in the following abstract Cauchy problem.

In the following we deal with the abstract Cauchy Problem for the simplified model.

3.1.1 Abstract Cauchy problem: Transport model for the neutrons

We have a Banach space $\mathbf{X} := L^1(S \times V)$ with Lebesgue measure on $S \times V \subset \mathbb{R}^6$ and define the abstract Cauchy problem as:

$$\frac{du(t)}{dt} = Bu(t), \quad (7)$$

$$\frac{du(t)}{dt} = (A_0 - M_\sigma + K_\kappa)u(t), \quad (8)$$

$$u(0) = u_0, \quad (9)$$

where $u \in \mathbf{X}$.

We have the following operators:

- 1.) Collision-less transport operator
- 2.) Absorption operator
- 3.) Scattering Operator

An important results for further numerical analysis is the fact, that the transport semi-group can be estimated by an exponential growth, see [4]:

Corollary 3.1. *We assume that $s(B) > -\infty$ is a dominant eigenvalue and $(S(t))_{t \geq 0}$ is irreducible. Then the transport semi-group $(S(t))_{t \geq 0}$ has balanced exponential growth. There exists a one-dimensional projection P satisfying $0 < P f$ whenever $0 < f$ such that:*

$$\|\exp(-s(B)t)S(t) - P\| \leq M \exp(-\epsilon t), \quad (10)$$

for all $t \geq 0$ and appropriate $M \geq 1$ and $\epsilon > 0$.

3.2 Transport model for the electrons or ions

For this model we can assume that $f(x, v, t)$ describe the density distribution of particles at position $x \in S$ with speed $v \in V$ at time $t \in [0, T]$, see also [4] and [17].

The space S is assumed to be a compact and convex subset of \mathbb{R}^3 with nonempty interior, and the velocity space V is:

$$V := \{v \in \mathbb{R}^3 : v_{min} \leq ||v||_2 \leq v_{max}\}$$

for $v_{min} > 0$ and $v_{max} < \infty$.

Assumption 3.2. *We have the following assumptions:*

- *Particles move according to their speed v .*
- *Particles are absorbed with function σ (e.g. probability function), depending on x and v .*
- *Particles are scattered to a scattering kernel κ depending on position x , incoming speed v' and outgoing speed v .*
- *Particles are influenced by the static electric field ϕ , which can be derived by the kinetic theory.*

The electron transport is given as:

$$\begin{aligned} \frac{\partial f(x, v, t)}{\partial t} &= -v \cdot \nabla_x f(x, v, t) - \frac{e}{m_e} \nabla_x \phi \cdot \nabla_v f(x, v, t) \\ &\quad - \sigma(x, v, t) f(x, v, t) + \int_V \kappa(x, v, v') f(x, v', t) dv', \end{aligned} \quad (11)$$

$$f(x, v, 0) = f_0(x, v), \quad (12)$$

and boundary conditions are included in the transport operators. ϕ is the electric field.

Further we have the Poisson's equation:

$$-\nabla_x \cdot (\epsilon \nabla \phi) = \begin{cases} e(n_i - \int_0^f dS) & \text{in } P \\ 0 & \text{in } D \end{cases}, \quad (13)$$

the permittivity is equal to ϵ_0 in the plasma P and $\epsilon_0 \epsilon_D$ in the dielectric D .

$$\begin{aligned} \frac{\partial f(x, v, t)}{\partial t} &= -v \cdot \nabla_x f(x, v, t) - \nabla_x D \cdot \nabla_x f(x, v, t) \\ &\quad - \sigma(x, v, t) f(x, v, t) + \int_V \kappa(x, v, v') f(x, v', t) dv', \end{aligned} \quad (14)$$

$$f(x, v, 0) = f_0(x, v), \quad (15)$$

and boundary conditions are included in the transport operators A_0 and A_1 see in the following abstract Cauchy problem. D is the diffusion parameter that includes the electric field.

Next we deal with the abstract Cauchy Problem for the simplified model.

3.2.1 Abstract Cauchy problem: Transport model for the neutrons

We have a Banach space $\mathbf{X} := L^1(S \times V)$ with Lebesgue measure on $S \times V \subset \mathbb{R}^6$ and define the abstract Cauchy problem as:

$$\frac{du(t)}{dt} = Bu(t), \quad (16)$$

$$\frac{du(t)}{dt} = (A_0 + A_1 - M_\sigma + K_\kappa)u(t), \quad (17)$$

$$u(0) = u_0, \quad (18)$$

where $u \in \mathbf{X}$.

We have the following operators:

- 1.) Collision-less transport operator
- 2.) Diffusion operator
- 3.) Absorption operator
- 4.) Scattering Operator

An important results for further numerical analysis is the fact, that the transport semi-group can be estimated by an exponential growth.

Corollary 3.2. *We assume that $s(B) > -\infty$ is a dominant eigenvalue and $(S(t))_{t \geq 0}$ is irreducible. Then the transport semi-group $(S(t))_{t \geq 0}$ has balanced exponential growth. There exists a one-dimensional projection P satisfying $0 < Pf$ whenever $0 < f$ such that:*

$$\|\exp(-s(B)t)S(t) - P\| \leq M \exp(-\epsilon t), \quad (19)$$

for all $t \geq 0$ and appropriate $M \geq 1$ and $\epsilon > 0$.

In the next section we discuss the splitting schemes.

4 Splitting schemes

The operator-splitting methods are used to solve complex models in the geophysical and environmental physics, they are developed and applied in [19], [20] and [21]. This ideas based in this article are solving simpler equations with respect to receive higher order discretization methods for the remain equations. For this aim we use the operator-splitting method and decouple the equation as follows described.

4.1 Splitting methods of first order for linear equations

First we describe the simplest operator-splitting, which is called β for the following system of ordinary linear differential equations:

$$\partial_t c(t) = A c(t) + B c(t), \quad (20)$$

whereby the initial-conditions are $c^n = c(t^n)$. The operators A and B are spatially discretized operators, e.g. they correspond to the discretized in space convection and diffusion operators (matrices). Hence, they can be considered as bounded operators.

The sequential operator-splitting method is introduced as a method which solve the two sub-problems sequentially, where the different sub-problems are connected via the initial conditions. This means that we replace the original problem (20) with the sub-problems

$$\begin{aligned} \frac{\partial c^*(t)}{\partial t} &= A c^*(t), \quad \text{with } c^*(t^n) = c^n, \\ \frac{\partial c^{**}(t)}{\partial t} &= B c^{**}(t), \quad \text{with } c^{**}(t^n) = c^*(t^{n+1}), \end{aligned} \quad (21)$$

whereby the splitting time-step is defined as $\tau_n = t^{n+1} - t^n$. The approximated split solution is defined as $c^{n+1} = c^{**}(t^{n+1})$.

Clearly, the change of the original problems with the sub-problems usually results some error, called *splitting error*. Obviously, the splitting error of the β

method can be derived as follows (cf. e.g.[12])

$$\begin{aligned}\rho_n &= \frac{1}{\tau}(\exp(\tau_n(A+B)) - \exp(\tau_n B) \exp(\tau_n A)) c(t^n) \\ &= \frac{1}{2}\tau_n[A, B] c(t^n) + O(\tau^2) .\end{aligned}\tag{22}$$

whereby $[A, B] := AB - BA$ is the commutator of A and B . Consequently, the splitting error is $O(\tau_n)$ when the operators A and B do not commute, otherwise the method is exact. Hence, by definition, the β is called *first order splitting method*.

4.2 Sequential splitting method for non-linear problems

We could use the result for the general formulation of nonlinear ordinary differential equations:

$$c'(t) = F_1(t, c(t)) + F_2(t, c(t)) ,\tag{23}$$

where the initial-conditions are given as $c^n = c(t^n)$.

As before, we can decouple the above problem into two (typically simpler) sub-problems, namely

$$\begin{aligned}\frac{\partial c^*(t)}{\partial t} &= F_1(t, c^*(t)) \text{ with } t^n \leq t \leq t^{n+1} \text{ and } c^*(t^n) = c^n , \\ \frac{\partial c^{**}(t)}{\partial t} &= F_2(t, c^{**}(t)) \text{ with } t^n \leq t \leq t^{n+1} \text{ and } c^{**}(t^n) = c^*(t^{n+1}) ,\end{aligned}\tag{24}$$

where the initial-values are given as $c^n = c(t^n)$ and the split approximation on the next time level is defined as $c^{n+1} = c^{**}(t^{n+1})$.

For this case the splitting error can be defined by use of the Jacobians of the non-linear mappings F_1 and F_2 , namely as

$$\rho_n = \frac{1}{2}\tau[\frac{\partial F_1}{\partial c}F_2, \frac{\partial F_2}{\partial c}F_1](t^n, c(t^n)) + O(\tau_n^2) .\tag{26}$$

Hence, for the general case the splitting error has of first order, i.e. $O(\tau_n)$.

4.3 Higher order splitting methods for linear operators

So far we defined the β which has first order accuracy. However in the practical computations in many cases we require splittings of higher order accuracy.

4.3.1 Symmetrically weighted sequential splitting.

In the following we introduce a weighted sequential splitting method, which is based on two sequential splitting methods with different ordering of the operators. I.e. we consider again the Cauchy problem (20) and we define the

operator-splitting on the time interval $[t^n, t^{n+1}]$ (where $t^{n+1} = t^n + \tau_n$) as follows

$$\begin{aligned} \frac{\partial c^*(t)}{\partial t} &= Ac^*(t) , \quad \text{with } c^*(t^n) = c^n , \\ \frac{\partial c^{**}(t)}{\partial t} &= Bc^{**}(t) , \quad \text{with } c^{**}(t^n) = c^*(t^{n+1}) . \end{aligned} \quad (27)$$

and

$$\begin{aligned} \frac{\partial v^*(t)}{\partial t} &= Bv^*(t) , \quad \text{with } v^*(t^n) = c^n , \\ \frac{\partial v^{**}(t)}{\partial t} &= Av^{**}(t) , \quad \text{with } v^{**}(t^n) = v^*(t^{n+1}) . \end{aligned} \quad (28)$$

where c^n is known.

Then the approximation at the next time-level t^{n+1} is defined as

$$c^{n+1} = \frac{c^{**}(t^{n+1}) + v^{**}(t^{n+1})}{2} \quad (29)$$

The splitting error of this operator splitting method is derived as follows (cf. [3])

$$\begin{aligned} \rho_n &= \frac{1}{\tau_n} \{ \exp(\tau_n(A+B)) - \frac{1}{2} [\exp(\tau_n B) \exp(\tau_n A) + \exp(\tau_n A) \exp(\tau_n B)] \} c(t^n) \\ &= O(\tau^2) . \end{aligned} \quad (30)$$

An easy computation shows that in general case the splitting error of this method is $O(\tau^2)$, i.e. the method is of second order accurate. (We note that in the case of commuting operators A and B the method is exact, i.e. the splitting error vanishes.)

4.3.2 Strang-Marchuk splitting method.

One of the most popular and widely used operator-splittings is the so-called *Strang splitting* (or *Strang-Marchuk splitting*), defined as follows [15, 19]. The methods reads as follows

$$\begin{aligned} \frac{\partial c^*(t)}{\partial t} &= Ac^*(t) , \quad \text{with } t^n \leq t \leq t^{n+1/2} \text{ and } c^*(t^n) = c^n , \\ \frac{\partial c^{**}(t)}{\partial t} &= Bc^{**}(t) , \quad \text{with } t^n \leq t \leq t^{n+1} \text{ and } c^{**}(t^n) = c^*(t^{n+1/2}) , \\ \frac{\partial c^{***}(t)}{\partial t} &= Ac^{***}(t) , \quad \text{with } t^{n+1/2} \leq t \leq t^{n+1} \text{ and } c^{***}(t^{n+1/2}) = c^{**}(t^{n+1}) , \end{aligned} \quad (31)$$

where $t^{n+1/2} = t^n + 0.5\tau_n$ and the approximation on the next time level t^{n+1} is defined as $c^{n+1} = c^{***}(t^{n+1})$.

The splitting error of the Strang splitting is

$$\rho_n = \frac{1}{24}(\tau_n)^2([B, [B, A]] - 2[A, [A, B]]) c(t^n) + O(\tau_n^4). \quad (32)$$

(See, e.g. ([10].) This means that this operator-splitting is of second order, too. (We note that under some special conditions for the operators A and B , the Strang splitting has third order accuracy and even can be exact [5].)

In our application the first order splitting for the convection-reaction- and the diffusion-dispersion-term are applied, because of the dominance of the space-error. The time-error for this combination was only a constant in the total error.

In the next subsection we present the iterative-splitting method.

4.4 Iterative splitting method

The following algorithm is based on the iteration with fixed splitting discretization step-size τ , namely, on the time interval $[t^n, t^{n+1}]$ we solve the following sub-problems consecutively for $i = 0, 2, \dots, 2m$. (Cf. [13] and [9].)

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n \quad (33)$$

$$\text{and } c_0(t^n) = c^n, \quad c_{-1} = 0.0,$$

$$\frac{\partial c_{i+1}(t)}{\partial t} = Ac_i(t) + Bc_{i+1}(t), \quad (34)$$

$$\text{with } c_{i+1}(t^n) = c^n,$$

where c^n is the known split approximation at the time level $t = t^n$. The split approximation at the time-level $t = t^{n+1}$ is defined as $c^{n+1} = c_{2m+1}(t^{n+1})$. (Clearly, the function $c_{i+1}(t)$ depends on the interval $[t^n, t^{n+1}]$, too, but, for the sake of simplicity, in our notation we omit the dependence on n .)

In the following we will analyze the convergence and the rate of the convergence of the method (33)–(34) for m tends to infinity for the linear operators $A, B : \mathbf{X} \rightarrow \mathbf{X}$ where we assume that these operators and their sum are generators of the C_0 semi-groups. We emphasize that these operators aren't necessarily bounded, so, the convergence is examined in general Banach space setting.

Theorem 4.1. *Let us consider the abstract Cauchy problem in a Banach space \mathbf{X}*

$$\begin{aligned} \partial_t c(t) &= Ac(t) + Bc(t), \quad 0 < t \leq T \\ c(0) &= c_0 \end{aligned} \quad (35)$$

where $A, B, A+B : \mathbf{X} \rightarrow \mathbf{X}$ are given linear operators being generators of the C_0 -semi-group and $c_0 \in \mathbf{X}$ is a given element. Then the iteration process (33)–(34) is convergent and the rate of the convergence is of second order.

Proof. Let us consider the iteration (33)–(34) on the sub-interval $[t^n, t^{n+1}]$. For the error function $e_i(t) = c(t) - c_i(t)$ we have the relations

$$\begin{aligned} \partial_t e_i(t) &= A e_i(t) + B e_{i-1}(t), \quad t \in (t^n, t^{n+1}], \\ e_i(t^n) &= 0 \end{aligned} \quad (36)$$

and

$$\begin{aligned} \partial_t e_{i+1}(t) &= A e_i(t) + B e_{i+1}(t), \quad t \in (t^n, t^{n+1}], \\ e_{i+1}(t^n) &= 0 \end{aligned} \quad (37)$$

for $m = 0, 2, 4, \dots$, with $e_0(0) = 0$ and $e_{-1}(t) = c(t)$. In the following we use the notations \mathbf{X}^2 for the product space $\mathbf{X} \times \mathbf{X}$ enabled with the norm $\|(u, v)\| = \max\{\|u\|, \|v\|\}$ ($u, v \in \mathbf{X}$). The elements $\mathcal{E}_i(t), \mathcal{F}_i(t) \in \mathbf{X}^2$ and the linear operator $\mathcal{A} : \mathbf{X}^2 \rightarrow \mathbf{X}^2$ are defined as follows

$$\mathcal{E}_i(t) = \begin{bmatrix} e_i(t) \\ e_{i+1}(t) \end{bmatrix}; \quad \mathcal{F}_i(t) = \begin{bmatrix} e_{i-1}(t) \\ 0 \end{bmatrix}; \quad \mathcal{A} = \begin{bmatrix} A & 0 \\ A & B \end{bmatrix}. \quad (38)$$

Then, using the notations (38), the relations (78)–(37) can be written in the form

$$\begin{aligned} \partial_t \mathcal{E}_i(t) &= \mathcal{A} \mathcal{E}_i(t) + \mathcal{F}_i(t), \quad t \in (t^n, t^{n+1}], \\ \mathcal{E}_i(t^n) &= 0. \end{aligned} \quad (39)$$

Due to our assumptions, \mathcal{A} is a generator of the one-parameter C_0 semi-group $(\mathcal{A}(t))_{t \geq 0}$, hence using the variations of constants formula, the solution of the abstract Cauchy problem (39) with homogeneous initial condition can be written as

$$\mathcal{E}_i(t) = \int_{t^n}^t \exp(\mathcal{A}(t-s)) \mathcal{F}_i(s) ds, \quad t \in [t^n, t^{n+1}]. \quad (40)$$

(See, e.g. [4].) Hence, using the denotation

$$\|\mathcal{E}_i\|_\infty = \sup_{t \in [t^n, t^{n+1}]} \|\mathcal{E}_i(t)\| \quad (41)$$

we have

$$\begin{aligned} \|\mathcal{E}_i\|(t) &\leq \|\mathcal{F}_i\|_\infty \int_{t^n}^t \|\exp(\mathcal{A}(t-s))\| ds = \\ &= \|e_{i-1}\| \int_{t^n}^t \|\exp(\mathcal{A}(t-s))\| ds, \quad t \in [t^n, t^{n+1}]. \end{aligned} \quad (42)$$

Since $(\mathcal{A}(t))_{t \geq 0}$ is a semi-group therefore the so called *growth estimation*

$$\|\exp(\mathcal{A}t)\| \leq K \exp(\omega t); \quad t \geq 0 \quad (43)$$

holds with some numbers $K \geq 0$ and $\omega \in \mathbb{R}$ [4].

- Assume that $(\mathcal{A}(t))_{t \geq 0}$ is a bounded or exponentially stable semi-group, i.e. (43) holds with some $\omega \leq 0$. Then obviously the estimate

$$\|\exp(\mathcal{A}t)\| \leq K; \quad t \geq 0 \quad (44)$$

holds, and, hence on base of (78), we have the relation

$$\|\mathcal{E}_i\|(t) \leq K\tau_n\|e_{i-1}\|, \quad t \in (0, \tau_n). \quad (45)$$

- Assume that $(\mathcal{A}(t))_{t \geq 0}$ has an exponential growth with some $\omega > 0$. Using (78) we have

$$\int_{t^n}^{t^{n+1}} \|\exp(\mathcal{A}(t-s))\| ds \leq K_\omega(t), \quad t \in [t^n, t^{n+1}], \quad (46)$$

where

$$K_\omega(t) = \frac{K}{\omega} (\exp(\omega(t-t^n)) - 1), \quad t \in [t^n, t^{n+1}]. \quad (47)$$

Hence

$$K_\omega(t) \leq \frac{K}{\omega} (\exp(\omega\tau_n) - 1) = K\tau_n + \mathcal{O}(\tau_n^2) \quad (48)$$

The estimations (45) and (48) result in that

$$\|\mathcal{E}_i\|_\infty = K\tau_n\|e_{i-1}\| + \mathcal{O}(\tau_n^2). \quad (49)$$

Taking into the account the definition of \mathcal{E}_i and the norm $\|\cdot\|_\infty$, we obtain

$$\|e_i\| = K\tau_n\|e_{i-1}\| + \mathcal{O}(\tau_n^2), \quad (50)$$

and hence

$$\|e_{i+1}\| = K_1\tau_n^2\|e_{i-1}\| + \mathcal{O}(\tau_n^3), \quad (51)$$

which proves our statement. \square

Remark 4.1. When A and B are matrices (i.e. (33)–(34) is a system of the ordinary differential equations), for the growth estimation (43) we can use the concept of the logarithmic norm. (See e.g.[11].) Hence, for many important class of matrices we can prove the validity of (43) with $\omega \leq 0$.

Remark 4.2. We note that a huge class of important differential operators generate contractive semi-group. This means that for such problems -assuming the exact solvability of the split sub-problems- the iterative splitting method is convergent in second order to the exact solution.

Modify to :

$$\frac{\partial c^i(t)}{\partial t} = Ac^i(t) + Bc^{i-1}(t), \text{ with } c^i(t^n) = c^{i-1}(t^{n+1}) \quad (52)$$

and the starting values $c^0(t^n) = c(t^n)$ results of last iteration , $c^{-1}(t^n) = 0.0$,

$$\frac{\partial c^{i+1}(t)}{\partial t} = Ac^i(t) + Bc^{i+1}(t), \quad (53)$$

with $c^{i+1}(t^n) = c^i(t^{n+1})$,

$$\epsilon > |c^{i+1}(t^{n+1}) - c^{i-1}(t^{n+1})| \text{Stop criterion} \quad (54)$$

$$\text{result for the next time-step} \quad (55)$$

$$c(t^{n+1}) = c^n(t^{n+1}), \text{ for } m \text{ fulfill the stop-criterion} \quad (56)$$

for each $i = 0, 2, \dots$, where c^n is the known split approximation at the previous time level.

5 Numerical Integration of the Integro-Part

We deal with the following integro-differential equation:

$$\frac{\partial u}{\partial t} = \int_0^t u(s) ds, \quad (57)$$

$$u(0) = u_0, \quad (58)$$

The integration part is done numerically with:

Trapezoidal rule:

$$\int_a^b f(x) dx \approx \frac{b-a}{n} \left(\frac{f(a) + f(b)}{2} + \sum_{k=1}^{n-1} f\left(a + k \frac{b-a}{n}\right) \right) \quad (59)$$

where the sub-intervals have the form $[kh, (k+1)h]$, with $h = (b-a)/n$ and $k = 0, 1, 2, \dots, n-1$.

The higher order formulas are given as closed NewtonCotes formulas are given as

where f_i is a shorthand for $f(x_i)$, with $x_i = a + i(b-a)/n$, and n the degree.

We obtain the following formulas for the Trapezoidal-rule:

$$\frac{\partial u}{\partial t} = t/2(u(0) + u(t)) ds, \quad (60)$$

$$u(0) = u_0, \quad (61)$$

and obtain the analytical result:

$$u(t) = \frac{2}{3} \exp\left(\frac{t^2}{4}\right)u(0) - \frac{1}{3}u(0), \quad (62)$$

Degree	Common name	Formula	Error term
1	Trapezoid rule	$\frac{b-a}{2}(f_0 + f_1)$	$-\frac{(b-a)^3}{12}f^{(2)}(\xi)$
2	Simpson's rule	$\frac{b-a}{6}(f_0 + 4f_1 + f_2)$	$-\frac{(b-a)^5}{2880}f^{(4)}(\xi)$
3	Simpson's 3/8 rule	$\frac{b-a}{8}(f_0 + 3f_1 + 3f_2 + f_3)$	$-\frac{(b-a)^5}{6480}f^{(4)}(\xi)$
4	Boole's rule	$\frac{b-a}{90}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4)$	$-\frac{(b-a)^7}{1935360}f^{(6)}(\xi)$

Table 1: Numerical Integration formulas (Closed NewtonCotes Formulas).

For the higher order formula like Simpsons-rule, we have the following results:

$$\frac{\partial u}{\partial t} = t/6(u(0) + 4u(t/2) + u(t)) \, ds, \quad (63)$$

$$u(0) = u_0, \quad (64)$$

We apply the idea of the polynomial solution:

$$u(t) = a_0 + a_1t + a_2t^2 + a_3t^3 + \dots$$

and we obtain the results with deriving the coefficients :

$$a_1 + 2a_2t + 3a_3t^2 + \dots \quad (65)$$

$$= t/6(a_0 + 4(a_0 + a_1t/2 + a_2t^2/4 + a_3t^3/8 + \dots) + a_0 + a_1t + a_2t^2 + a_3t^3 + \dots),$$

$$a_0 = u_0, \quad (66)$$

and we obtain via coefficient comparison:

$$a_0 = u_0 \quad (67)$$

$$a_1 = a_3 = a_5 = \dots = 0 \quad (68)$$

$$a_2 = 3a_0 \quad (69)$$

$$a_4 = \frac{1}{12}a_2, \dots, \quad (70)$$

Remark 5.1. Such fast algorithms of generalized Taylor series about a function (here we apply numerical integration formulas) are computed very efficient, see also the decomposition ideas of [1].

6 Experiments for the Plasma resonance spectroscopy

6.1 First Example: Matrix problem with integral term

We deal with a simpler integro-differential equations:

$$c'(t) = c + \int_0^t c(t)dt, \quad t \in [0, 1], \quad (71)$$

where we assume $\int_0^t c(t)dt = tc(t)$ as a first order approximation of the integral and deal with:

$$c'(t) = c + tc(t), \quad t \in [0, T], \quad (72)$$

$$c(0) = c(t_0) = 1, \quad (73)$$

where $T = 10.0$ and we have the analytical solution for the approximation which is given as:

$$c(t) = \exp\left(t + \frac{t^2}{2}\right)u(0), \quad (74)$$

We split into:

$$A = 1, \quad (75)$$

$$B(t) = t, \quad (76)$$

We have the following solutions for the iterative scheme:

$$c_1(t) = \exp(A(t^{n+1} - t))c(t^n), \quad t \in (t^n, t^{n+1}], \quad (77)$$

$$\begin{aligned} c_2(t) &= \exp\left(\int_{t^n}^{t^{n+1}} B(t)dt\right)c(t^n) \\ &+ \int_{t^n}^{t^{n+1}} \exp\left(\int_s^{t^{n+1}} B(t^{n+1} - t)dt\right)Ac_1(s)ds, \quad t \in (t^n, t^{n+1}]. \end{aligned} \quad (78)$$

where $n = 0, 1, \dots, N$ and $t^N = T$ while the time-steps are given as $\Delta t = t^{n+1} - t^n$.

We deal with the following recurrence relations with even and odd iterations:

for the odd iterations: $i = 2m + 1$,

for $m = 0, 1, 2, \dots$

$$\begin{aligned} c_i(t) &= \exp(A(t - t^n))c(t^n) \\ &+ \int_{t^n}^t \exp(sA)B(s)c_{i-1}(t^{n+1} - s)ds, \quad t \in (t^n, t^{n+1}]. \end{aligned} \quad (79)$$

For the even iterations: $i = 2m$,

for $m = 1, 2, \dots$

$$\begin{aligned} c_i(t) &= \exp\left(\int_{t^n}^{t^{n+1}} B(s)ds\right)c(t^n) \\ &+ \int_{t^n}^t \exp\left(\int_0^s B(t)dt\right)Ac_{i-1}(t^{n+1} - s)ds, \quad t \in (t^n, t^{n+1}]. \end{aligned} \quad (80)$$

In the table 2 we obtain the numerical results of the iterative splitting scheme.

In the Figure 1, we present the one-side and two-side iterative results.

Remark 6.1. *In the experiments, we obtain improved results with each additional step. By the way the solution blows up and we have to use also very fine time-steps to control the errors. Optimal results are obtain by using the integral part (stiff part) as the implicit part in the iteration (one-side over B).*

	$\Delta t=1$	$\Delta t=0.5$	$\Delta t=0.25$	$\Delta t=2^{-3}$	$\Delta t=2^{-4}$
c_1	1.7634	0.4958	0.1793	0.0753	0.0343
c_2	0.8628	0.1444	0.0282	0.0061	0.0014
c_3	0.2220	0.0104	5.2127e-04	2.8455e-05	1.6511e-06
c_4	0.1116	0.0041	1.8660e-04	9.7846e-06	5.5769e-07
c_5	0.0971	0.0039	1.8367e-04	9.7418e-06	5.5644e-07
c_6	0.0956	0.0039	1.8365e-04	9.7418e-06	5.5644e-07
c_7	0.0954	0.0039	1.8365e-04	9.7416e-06	5.5644e-07
c_8	0.0954	0.0039	1.8366e-04	9.7343e-06	5.5556e-07

Table 2: Numerical experiment with 10 iterative steps for the first example.

6.2 Real-life problem

In the following subsections, we present our experiments based on the neutron transport.

A simplified one-dimensional model is given as:

$$\partial_t c + v \partial_x c - D \partial_{xx} c + \sigma c = \int_{\Omega} \kappa(x, v, v') c(x, v', t) dv',$$

The velocity v and the diffusion D is given by the plasma model. The initial conditions are given by $c(x, 0) = c_0(x)$ and the boundary conditions are trivial $\partial_n c(x, t) = 0$.

A first integral operator is given as:

$$\int_{\Omega} \kappa(x, v, v') c(x, v', t) dv' = \int_0^T c(x, t) dt,$$

A second integral operator is given as:

We assume a simple collision operator: $\kappa(x, v, v') = q(v')(1 + v'^2)$ where $q(v')$ is the potential, $e.g. v'^2$.

We deal with the first integral operator and define the following operators:

$$A = v \frac{1}{\Delta x} [1 - 1] I - D \frac{1}{\Delta x^2} [1 - 21] I$$

$$B = (-\sigma + t) I$$

while

$$\exp(Bt) = \exp((- \sigma t + t^2/2) I)$$

where I is the identity matrix of rank.

6.2.1 One phase example

The next example is a simplified real-life problem for a neutron transport equation, which includes the gain and loss of a neutron

We concentrate on the computational benefits of a fast computation of the iterative scheme, given with matrix exponentials.

The equation is given as:

$$\partial_t c + \nabla \cdot \mathbf{F}c = -\lambda_1 c + \int_0^t \lambda_2 c(x, t) dt, \text{ in } \Omega \times [0, t], \quad (81)$$

$$\mathbf{F} = \mathbf{v} - D\nabla, \quad (82)$$

$$c(\mathbf{x}, t) = c_0(\mathbf{x}), \text{ on } \Omega, \quad (83)$$

$$c(\mathbf{x}, t) = c_1(\mathbf{x}, t), \text{ on } \partial\Omega \times [0, t], \quad (84)$$

In the following we deal with the semi-discretized equation given with the matrices:

$$\partial_t \mathbf{C} = (A - \Lambda_1 + \Lambda_2) \mathbf{C}, \quad (85)$$

where $\mathbf{C} = (c_1, \dots, c_I)^T$ is the solution of the species in the mobile phase in each spatial discretization point ($i = 1, \dots, I$).

We have the following two operators for the splitting method:

$$A = \frac{D}{\Delta x^2} \cdot \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} \quad (86)$$

$$+ \frac{v}{\Delta x} \cdot \begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 & 1 \\ & & & -1 & 1 \end{pmatrix} \in \mathbb{R}^{I \times I} \quad (87)$$

where I is the number of spatial points.

$$\Lambda_1 = \begin{pmatrix} \lambda_1 & 0 & & \\ 0 & \lambda_1 & 0 & \\ & \ddots & \ddots & \ddots \\ & & 0 & \lambda_1 & 0 \\ & & & 0 & \lambda_1 \end{pmatrix} \in \mathbb{R}^{I \times I} \quad (88)$$

For the integral term we have the following ideas:

Case 1:

$$\int_0^t \lambda_2 c(x, t) dt \approx \lambda_2 t c(x, t)$$

and we obtain the Matrix:

$$\Lambda_2 = \begin{pmatrix} \lambda_2 t^2/2 & 0 & & & \\ & 0 & \lambda_2 t^2/2 & 0 & \\ & & \ddots & \ddots & \ddots \\ & & & 0 & \lambda_2 t^2/2 & 0 \\ & & & & 0 & \lambda_2 t^2/2 \end{pmatrix} \in \mathbb{R}^{I \times I} \quad (89)$$

For the operator splitting scheme we apply A and $B = -\Lambda_1 + \Lambda_2$ and we apply the iterative splitting method, given in equations (79)- (80).

Case 2:

We integrate the operator B with respect to the previous solutions \mathbf{C}_{i-1} and we obtain the Matrix:

$$\begin{aligned} & \Lambda_2(\mathbf{C}_{i-1}) \\ &= \begin{pmatrix} \int_0^t \lambda_2 c_{1,i-1}(x, s) ds & 0 & \dots & 0 \\ 0 & \int_0^t \lambda_2 c_{2,i-1}(x, s) ds & 0 & \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \int_0^t \lambda_2 c_{I,i-1}(x, s) ds \end{pmatrix} \\ & \in \mathbb{R}^{I \times I} \end{aligned} \quad (90)$$

We obtain $B(\mathbf{C}) = \Lambda_2(\mathbf{C}_{i-1}) + \Lambda_1 \mathbf{C}$

The iterative scheme is given as:

For $i = 1, 2, \dots$

$$\begin{aligned} \mathbf{C}_i(t) &= \exp(A(t - t^n))\mathbf{C}(t^n) \\ &+ \int_{t^n}^t \exp((t - s)A)B(\mathbf{C}_{i-1}(s)) ds, \quad t \in (t^n, t^{n+1}]. \end{aligned} \quad (91)$$

For the reference solution, we apply a fine time- and spatial scale without decoupling the equations.

The Figure 2 present the numerical errors between the exact and the numerical solution. Here we obtain optimal results for one-side iterative schemes on operator B , means we iterate with respect to B and use A as right hand side.

Remark 6.2. *For all iterative schemes, we can reach faster results as for the The iterative schemes with fast computations of the exponential matrices standard schemes. With 4 – 5 iterative steps we obtain more accurate results as we did for the expensive standard schemes. With one-side iterative schemes we reach the best convergence results.*

7 Conclusions and Discussions

We present the coupled model for a transport model for deposition species in a plasma environment. We assume the flow field is computed by the plasma model and the transport of the deposition species with a transport-reaction model.

Such a first model can help to understand the important modeling of the plasma environment in a CVD reactor.

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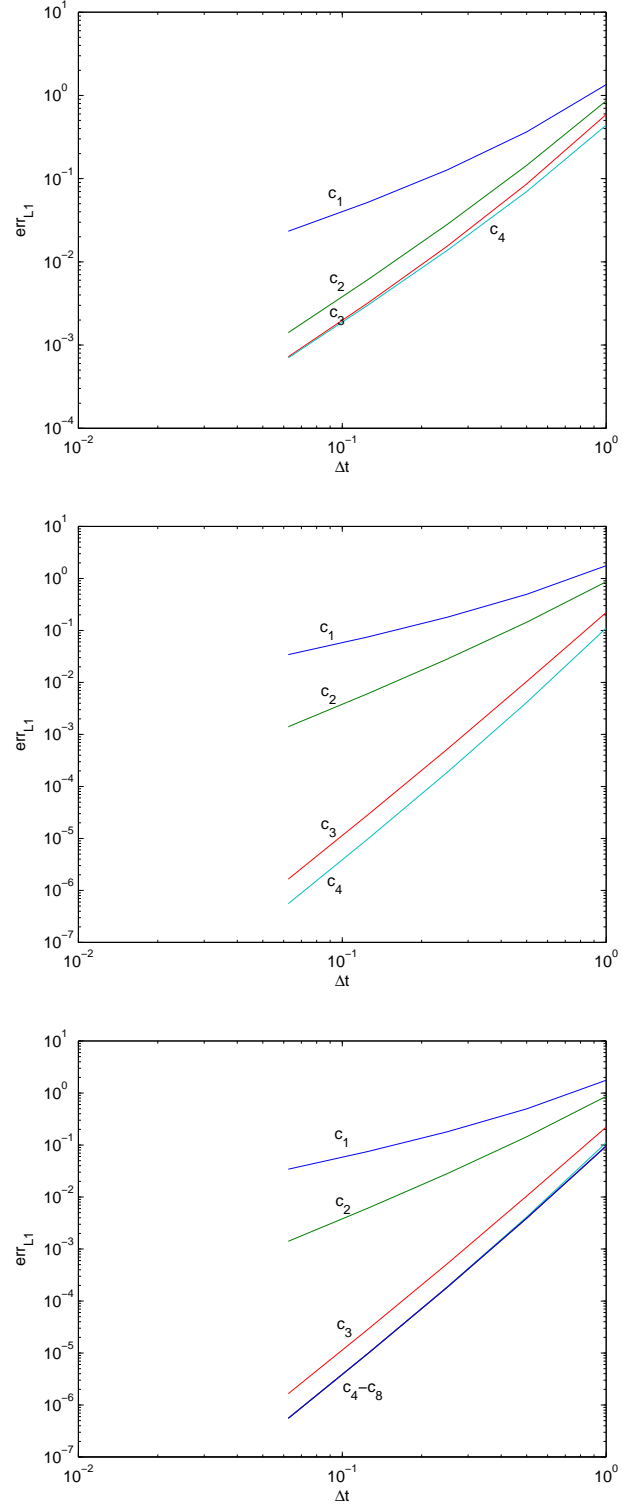


Figure 1: Numerical errors of the one-side and two-side Splitting scheme: one-side splitting over A (upper figure), one-side splitting over B (middle figure) and two-side splitting scheme alternating between A and B (lower figure) with $1, \dots, 8$ iterative steps.

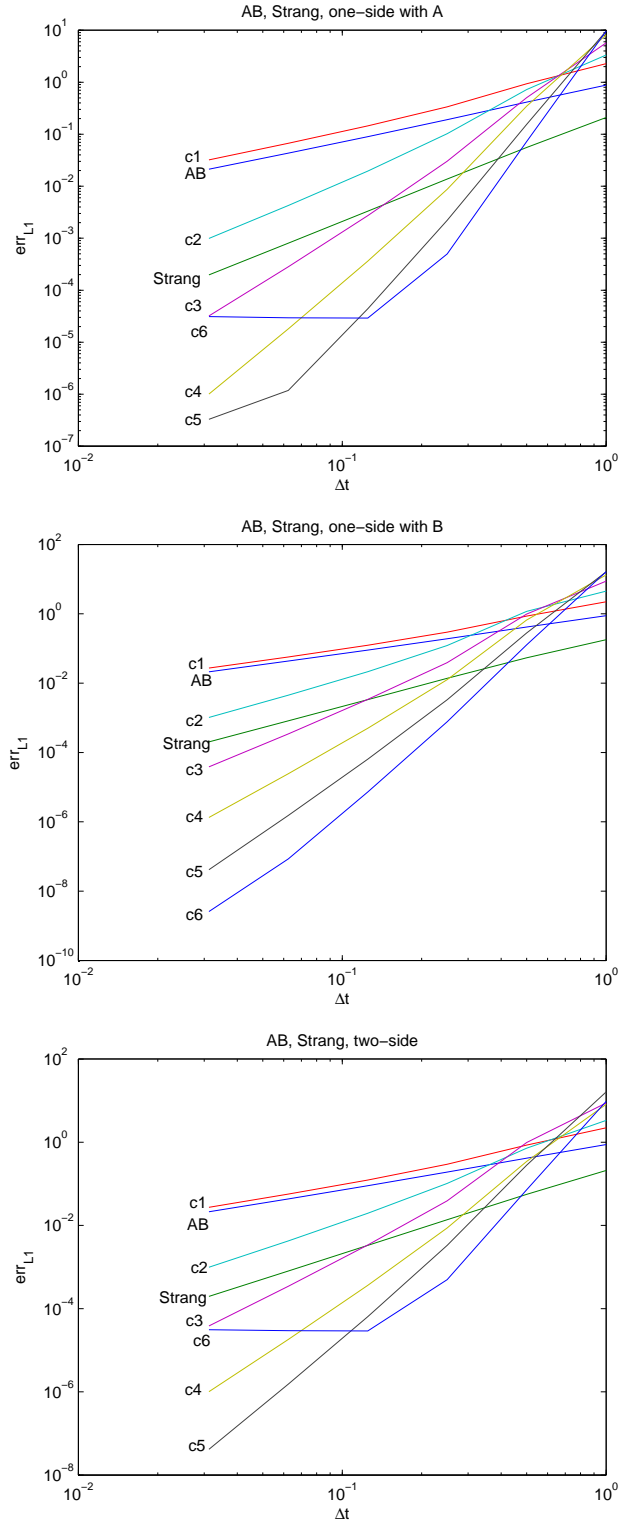


Figure 2: Numerical errors of the one-side Splitting scheme with A (upper figure), the one-side Splitting scheme with B (middle figure) and the iterative schemes with $1, \dots, 6$ iterative steps (lower figure).